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Microscopic Studies of Clusters in Phase Transitions

During the period 1 October 1990 to 30 September 1991 research was done on the following projects.

1. Droplet structure in nucleation near the spinodal singularity in liquid-gas like transitions

The structure of critical or nucleation droplets was studied in the proximity of the classical spinodal in Ising models. It was shown that the critical droplets could be described as a coalescence of clusters associated with the spinodal critical point fluctuations. The structure of these clusters could be determined by mapping the thermal spinodal singularity onto a percolation model. The linear size of these droplets or clusters was seen to be proportional to the thermal correlation length which diverges as the spinodal is approached.

The coalescence process can be predicted by a Becker Döring theory and was observed in computer simulations of Ising models. Understanding this process gives us new insight into the nucleation mechanism in the neighborhood of the classical spinodal for systems with long to moderate range interactions.

Publication 1

2. Clusters and symmetry in spinodal decomposition and continuous ordering

The phenomena of continuous ordering and spinodal decomposition are not well understood. The so-called linear theory or Cahn-Hilliard-Cook theory has a temporal range of validity that increases with interaction range but a description of the crossover to the non-linear regime as well as a reasonable theory for the early non-linear evolution is not available. In order to facilitate the development of such a theory we have begun to investigate the linear regime and its breakdown.

To that end we have mapped the linear regime of spinodal decomposition and continuous ordering onto a cluster growth problem, analyzed the fractal and mutifractal structures that appear and have begun to investigate the crossover to the non-linear behavior.

We have also investigated the existence of symmetries in the early stages of spinodal decomposition and continuous ordering and found that the linear or Cahn-Hilliard-Cook theory was characterized by the existence of supersymmetry which has a close connection with the cluster properties of the model.

Publication 2

3. Cluster acceleration algorithms

One of the major impediments to obtaining better numerical data on the kinetics of phase transitions is the time required to complete a run from the initial equilibrium state,

through the quench into the metastable or unstable state and finally to the new equilibrium state. The time constraints lead to simulations of small systems with the attendent finite size effects. In order to speed up the simulations we have begun to investigate the possible application of the new cluster acceleration algorithms introduced to study equilibrium critical phenomena to problems in the kinetics of phase transitions.

We have proposed an explanation of why the algorithms work as well as examining their dimensional dependence. We have also begun to investigate the generalization of these algorithms, constructed for systems with no conserved quantities, to models with a conserved order parameter.

In the final year of this effort we investigated the relation between the simulations we have performed and renormalization group (RG) calculations which appear to give different results. We concluded that the RG calculations were for a diffenent class of algorithms and that our original result was correct.

Publication 3

4. Effect of Perturbations on Critical Droplets.

We investigated the sensitivity of critical droplets to perturbations. The purpose was to understand the relation between the cluster structure representing the droplet and the evolution kinetics.

We found that the critical droplets were quite sensitive to perturbations but that classical droplets were most sensitive to purturbations on their surface while spinodal droplets were most sensitive in their interior.

Publication 4

Publications 1 October 1990 - 30 September 1991

1. L. Monette and W. Klein, Phys. Rev. Lett. **68**, 2336 (1992)
2. W. Klein and G. Batrouni, Phys. Rev. Lett. **67**, 1278 (1991)
3. P. Tamayo and W. Klein, Phys. Rev. Lett. **66**, 2049 (1991)
4. L. Monette, W. Klein, M. Zuckermann, J. Stat. Phys. **66**, 117 (1992)

Presentations of Supported Work

W. Klein

1. Invited Speaker-Minerals, Materials and Metals Society Oct. 1990
2. Seminar-McGill University, May 1991
3. Seminar-Exxon, June 1991
4. Seminar-Los Alamos, July 1991
5. Invited Speaker-Summer School on Chaos, Correlations and Complex Patterns, Copenhagen, Dennmark, August 1991
6. Seminar-Lawrence Livermore Laboratory, March 1992